

**Report on “Multiscale modeling of Semiconductor Nanostructures”
(Grant no. FA2386-09-1-4128)**

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Abstract

The main purpose of this proposal is to develop a new efficient method for multi-scale modeling of semiconductor nanostructures. Our approach provides a link between the *ab initio* method and the semi-empirical method based on continuum or tight-binding approach. The link is through the use of boundary-integrals involving Green's functions of separable domains. The method is most efficient when the system can be decomposed into two or more domains coupled through the interactions at the boundary (or boundaries) and the solution to each region (considered as extended to infinity) is obtainable either via *ab initio* method or semi-empirical method. Because the charge redistribution due to interaction at the boundaries remains localized near the interface(s), the Green's function approach will be extremely efficient. The method allows fast simulation of electronic states of nanostructures of realistic dimension (up to 30nm in cross-section) via semi-empirical method, while keep the salient features of interface electronic properties by treating the effect of charge transfer and atomic relaxation at interfaces via *ab initio* method.

Progress

The following research results based on empirical model and continuum model were published or submitted. (all funded by this grant).

1. Van der Waals Interaction between Two Crossed Carbon Nanotubes

[A. I. Zhbanov, E. G. Pogorelov, and Y.-C. Chang, ACS nano, **4**(10),5937-45 (2010).]

The analytical expressions for the van der Waals potential energy and force between two crossed carbon nanotubes are presented. The Lennard-Jones potential between pairs of carbon atoms and the smearedout approximation suggested by L. A. Girifalco (J. Phys. Chem. 1992, 96, 858) were used. The exact formula is expressed in terms of rational and elliptical functions. The potential and force for carbon nanotubes were calculated. The uniform potential curves for single- and multiwall nanotubes were plotted. The equilibrium distance, maximal attractive force, and potential energy have been evaluated.

2. Corrected field enhancement factor for the floating sphere model of carbon nanotube emitter

[E. G. Pogorelov, Y.-C. Chang, A. I. Zhbanov, and Y. G. Lee, J. Appl. Phys., **108**, 044502 (2010).]

We have corrected the field enhancement factor for the “floating sphere at emitter-plane potential” model with the finite anode-cathode distance. If r is the radius of sphere, h is the distance from cathode to the center of sphere, and l is the distance from the center to the anode, then the field enhancement factor is given as the following expression $\beta_{\text{sph}} = (2 + 7\eta - \eta^2)(\lambda^2 - 2\lambda + 2) / [2\eta(1 - \lambda)(2 - \lambda)]$, where $\eta = \rho/h$, $\lambda = \rho/l$. This expression demonstrates reasonable behavior for three limiting cases: if $h \rightarrow \rho$, if $l \rightarrow \infty$, and if $l \rightarrow \rho$. We have compared our factor β_{sph} with the field

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enhancement factor β_{tube} for the “hemisphere on a post” model and the factor β_{ell} for the “hemiellipsoid on plane” model. We have shown realization of the approximate evaluation $\beta_{\text{tube}} \sim (\beta_{\text{sph}} + \beta_{\text{ell}})/2$.

3. Comment on 'Model calculation of the scanned field enhancement factor of CNTs'

[A. I. Zhbanov, Y.-G. Lee, E. G. Pogorelov, Y.-C. Chang, Nanotechnology, **21**, 358001 (2010)]

The model proposed by Ahmad and Tripathi (2006 Nanotechnology 17 3798) demonstrates that the field enhancement factor of carbon nanotubes (CNTs) reaches a maximum at a certain length. Here, we show that this behavior should not occur and suggest our correction to this model.

4. Laser-induced breathing modes in metallic nanoparticles: A symmetric molecular dynamics study

[M. Y. Ng, Y. C. Chang*, J. Chem. Phys., **134**, 094116 (2011)]

A highly efficient simulation method based on molecular dynamics and group theory is adopted to investigate the laser-induced breathing oscillation of gold and silver nanospheres. Nanoparticles with size ranging from 5.8 to 46.2 nm are discussed. The effect due to laser-induced heating is modeled by a symmetric sudden expansion of the nanospheres by increasing the interatomic distances. A long-range empirical potential model which is capable of describing the phonon dispersion curves of noble metals in the full frequency range is established. Group theory is fully exploited to increase the computation efficiency, and the oscillation behavior of nanospheres of over 3×10^6 atoms can be simulated efficiently. Oscillation frequencies of nanospheres are obtained by calculating the Fourier transform of the velocity autocorrelation function. The breathing modes of nanospheres are identified as the excitation of A_{1g} modes with in-phase radial displacement of atoms in the nanospheres. The resulting oscillation spectra are in very good agreement with experimental data.

5. Screened field enhancement factor for the floating sphere model of a carbon nanotube array

[A. I. Zhbanov, E. G. Pogorelov, Y.-C. Chang, Y.-G. Lee, J. Appl. Phys, in press (2011)]

The screened field enhancement factor for a carbon nanotube (CNT) placed in a CNT array (which is reduced due to the screening effect) is derived based on the “floating sphere” model. We obtain an expression for the field enhancement factor for a CNT in the array as $\gamma = 3 + 2(1+\eta)/\{(2+\eta)[2\pi\alpha(2+\eta)\delta^2 + \eta]\}$, where ρ is the radius of sphere, h is the distance from cathode to the center of sphere, and D is the distance between the nearest spheres, $\eta = \rho/h$, $\delta = \rho/D$, and $\alpha = 1$ for square or $2/\sqrt{3}$ for hexagonal lattice made of CNTs. Explicit algebraic formulas for optimizing the distance between tubes, areal density of emitters, and the anode current are also obtained.

6. Universal curves for van der Waals interaction between single-wall carbon nanotubes

[Evgeny G. Pogorelov, A. I. Zhbanov, Y.-C. Chang, and S. Yang, (submitted to Langmuir)]

We report very simple and accurate algebraic expressions for the van der Waals (VDW) potentials and the forces between two parallel and crossed carbon nanotubes. The Lennard-Jones potential for two carbon atoms and the method of the smeared out approximation suggested

by L.A. Girifalco were used. It is found that interaction between parallel and crossed tubes are described by two universal curves for parallel and crossed configurations which do not depend on the van der Waals constants, angle between tubes, surface density of atoms and its nature, but only on dimensionless distance. The explicit functions for equilibrium VDW distances, well depths, and maximal attractive forces have been given. These results may be used as a guide for analysis of experimental data to investigate interaction between nanotubes of various natures.